

Lattice QCD Campaign

Robert Edwards



LQCD group & collaborators

JEFFERSON LAB

Jozef Dudek
Robert Edwards
Balint Joo
Kostas Orginos
David Richards
Andre Walker-Loud
Frank Winter

POSTDOCS & STUDENTS

Raul Briceno
David Wilson (ODU)
Christian Shultz (ODU)
Chris Bouchard (W&M)
Arjun Gambhir (W&M)

COLLABORATORS

Mike Peardon (Trinity)
Sinead Ryan (Trinity)
Nilmani Mathur (Tata)
Christopher Thomas (Cambridge)
Steve Wallace (U. Maryland)
Rajan Gupta (LANL)
Sergey Syritsyn (BNL)
Christopher Monahan (Utah)
Andreas Stathopoulos (W&M)

MESON SPECTRUM

PRL103 262001 (2009) $I = 1$
PRD82 034508 (2010) $I = 1, K^*$
PRD83 111502 (2011) $I = 0$
JHEP07 126 (2011) $c\bar{c}$
PRD88 094505 (2013) $I = 0$
JHEP05 021 (2013) D, D_s

BARYON SPECTRUM

PRD84 074508 (2011) $(N, \Delta)^*$
PRD85 054016 (2012) $(N, \Delta)_{\text{hyb}}$
PRD87 054506 (2013) $(N \dots \Xi)^*$
PRD90 074504 (2014) Ω_{ccc}^*
PRD91 094502 (2015) Ξ_{cc}^*

HADRON SCATTERING

PRD83 071504 (2011) $\pi\pi I = 2$
PRD86 034031 (2012) $\pi\pi I = 2$
PRD87 034505 (2013) $\pi\pi I = 1, \rho$
PRL113 182001 (2014) $\pi K, \eta K$
PRD91 054008 (2015) $\pi K, \eta K$
ARXIV: 1507.02599 $\pi\pi I = 1, \rho$

NUCLEI

PRD87 034506 (2013)
PRD90 094507 (2014)
PRL113 25001 (2014)
PRD91 114503 (2015)
ARXIV: 1506.05518
ARXIV: 1505.02411

DISTRIBUTIONS

PRD91 074513 (2015) OPE

“TECHNOLOGY”

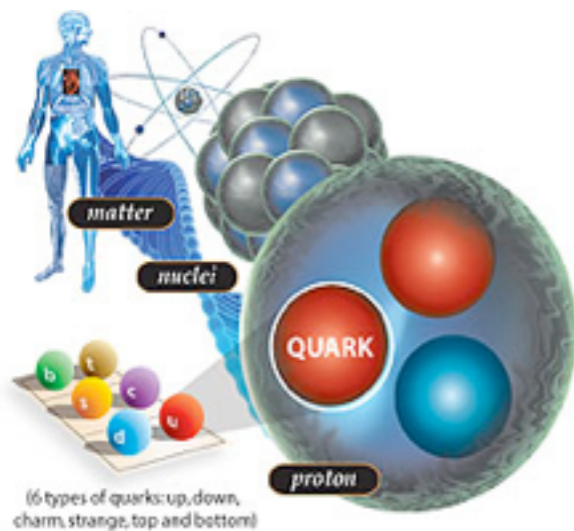
PRD79 034502 (2009) lattices
PRD80 054506 (2009) distillation
PRD85 014507 (2012) $\vec{p} > 0$

MATRIX ELEMENTS

PRD91 114501 (2015) $M' \rightarrow \gamma M$
PRD90 014511 (2014) f_{π^*}

Introduction

- Believe fundamental building blocks of matter are *quarks* bound by *gluons*, via *strong nuclear force*.
- Quantum Chromodynamics (QCD) - theory which describes the strong interactions
- Understanding how quarks and gluons constitute matter under QCD is a major expt. goal
 - < ~20% of proton mass comes from mass of the quarks, rest comes from glue
 - gluon self-coupling and gluon excitations can create *exotic forms of matter*



GlueX in the new Hall-D of Jefferson Lab@12 GeV. Hunting for exotics!

Jefferson Lab

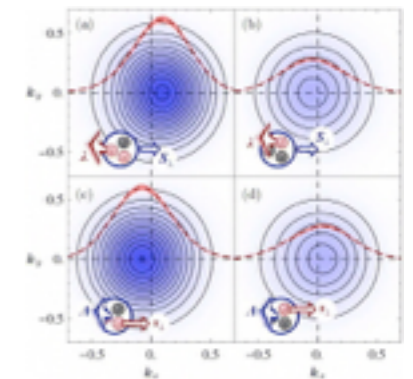
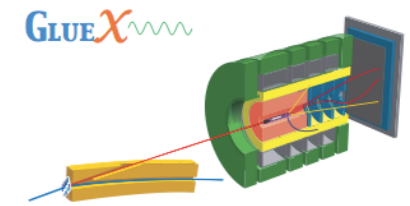


Brookhaven National Lab

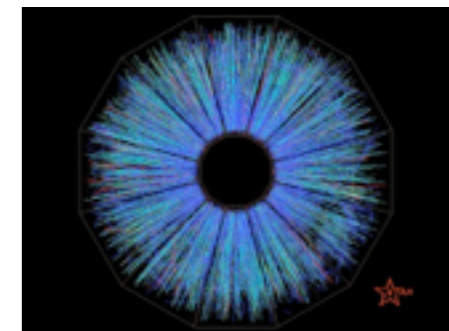
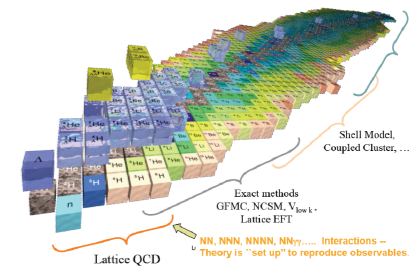


Questions in Nuclear Physics

- What observable states does QCD allow?
 - What is the role of the gluons? What about exotic matter?
 - Focus of GlueX experiment
- How do nucleons arise?
 - how are quarks & gluons distributed in a proton or neutron?
 - Focus of JLab 12 GeV, Halls A, B & C, RHIC-spin and future EIC
- QCD must predict properties of light nuclei
 - predict nuclear reaction properties, connect to effective theories
 - \$730M Facility for Rare Isotope Beam (FRIB) will investigate nuclear structure and interactions
- How does QCD behave under extreme temperatures & pressures such as in supernovae or shortly after Big-Bang
 - Studied in RHIC at BNL



Hägler, Musch, Negele, Schäfer, EPL 88 61001



USQCD National Effort

US Lattice QCD coordinated effort involving JLab, BNL & FNAL

USQCD Exec. Comm.

USQCD Sci. Prog. Comm.

Science campaigns:

HEP	Intensity Frontier
	Energy Frontier
NP	Cold nuclear physics
	Thermodynamics

USQCD Facilities:

2010 - 2014: LQCD ext: \$18M	}	\$23M
2009 - 2012: LQCD ARRA: \$5M		
<hr/>		
2015 - 2019: LQCD ext-II:		\$14M

Leadership Comp. Facilities:

Proposals to DOE + NSF programs
Resources: ORNL, ANL, NERSC, NSF

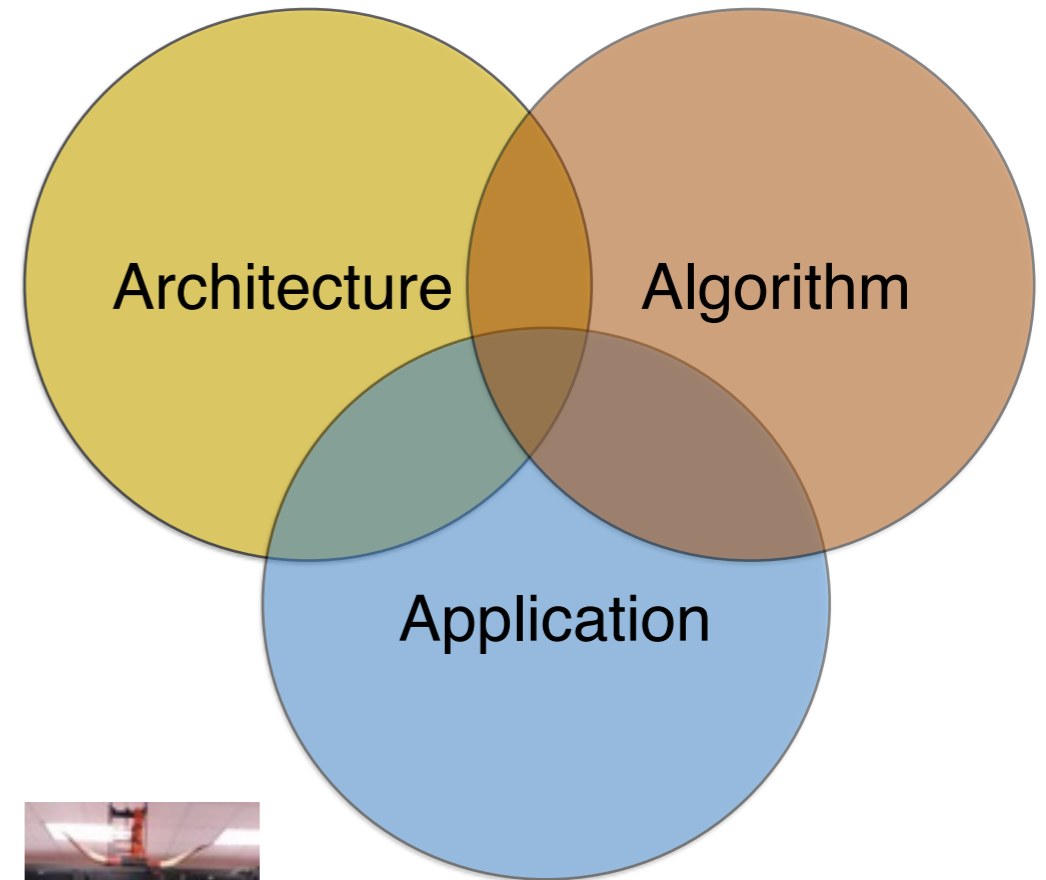
Software:

2001 - 2012: SciDAC I & II
2013 - 2016: HEP + ASCR SciDAC
2013 - 2016: NP + ASCR SciDAC
JLab portion: \$1.6M NP + \$0.88M ASCR

SciDAC

LQCD software development effort to support Leadership Computing and USQCD facilities

Applications	Chroma	CPS	MILC	FUEL	Qlua
Level 3	Solvers	MDWF	QOPQDP	QUDA	QphiX
Level 2	QDP++	QDP	QIO		
Level 1	QLA	QMP	QMT		

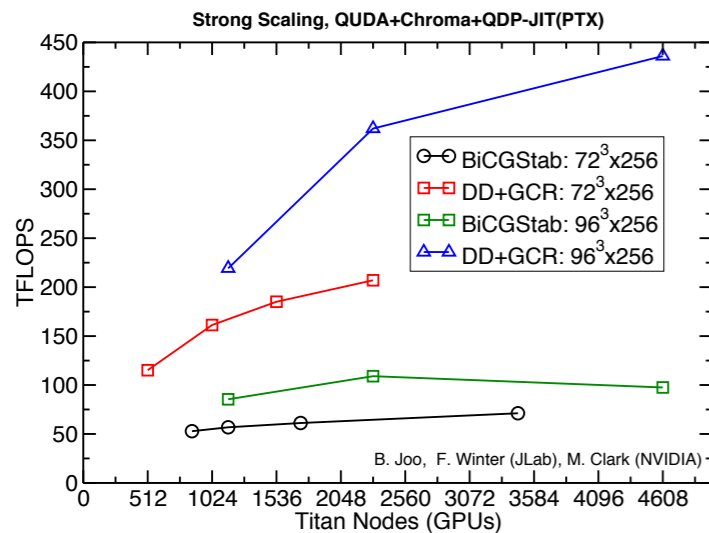


JLab: Jie Chen, Balint Joo, Frank Winter

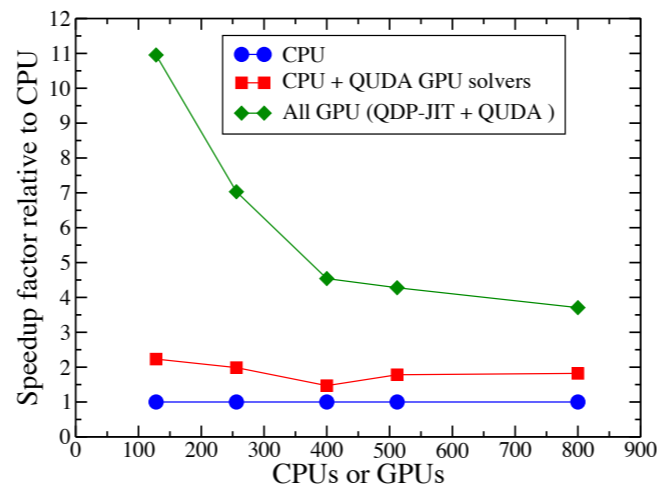
Many computing architectures

- Opportunity to optimize for speed & cost
 - Current & future leadership “*capability*” resources - gauge generation
 - USQCD “*capacity*” resources - propagators & contractions
- JLab has been at forefront of these developments
 - NviDIA GPUs (B. Joo, F. Winter + NviDIA developers)
 - Intel Many Core (Xeon Phi) (B. Joo, C. Watson + Intel Parallel Computing Labs)
 - BlueGene/Q (F. Winter + ANL staff)
 - Partnership with SciDAC Super Institute - “automatic” porting of code

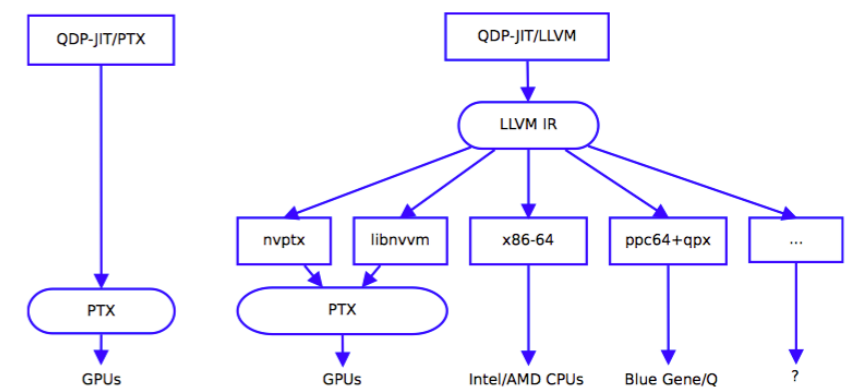
**Propagator speed
Titan (K20X)**



**Gauge generation speedups
Titan (K20X)**



**Porting code: Just-In-Time compilation
Domain specific language**



JLab + SciDAC Super Institute

Lattice QCD

- First-principles numerical approach to the field-theory

– Evaluate **correlation functions** e.g. $\int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}A_\mu \bar{\psi} \Gamma \psi(t) \bar{\psi} \Gamma \psi(0) e^{-\int d^4x \mathcal{L}_{\text{QCD}}(\psi, \bar{\psi}, A_\mu)}$
‘sum’ ‘field’ ‘probability’

via **Monte-Carlo** sampling of path-integral
on a **finite cubic grid**

» in principle recover physical QCD as

$$a \rightarrow 0 \quad L \rightarrow \infty$$

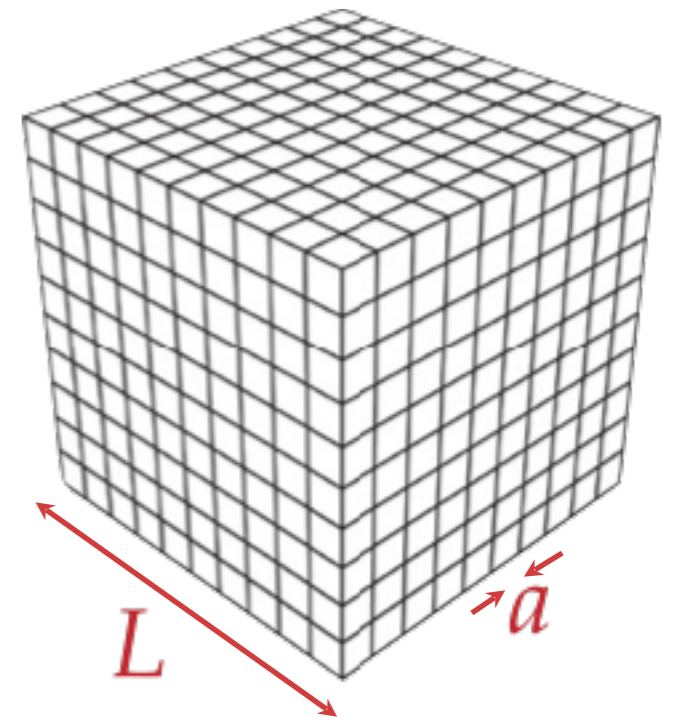
However, use finite L as a tool (see R. Briceno talk)

» practical calculations often use

$$m_q^{\text{calc.}} > m_q^{\text{phys.}}$$

» large scale computational problem ...

CUBIC LATTICE

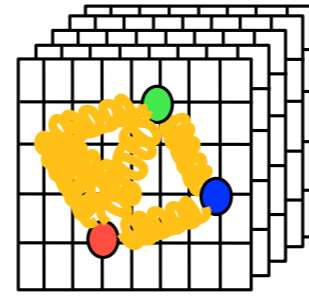
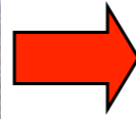


LQCD workflow

LQCD workflow

Generate the configurations

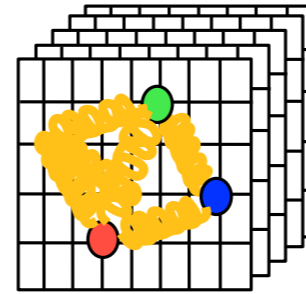
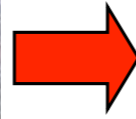
- Leadership level
- 60K cores, 10's TF-yr



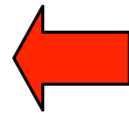
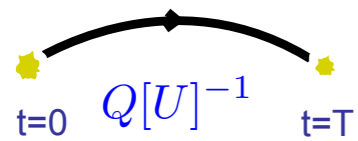
LQCD workflow

Generate the configurations

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Propagators



+



Analyze

- 100K copies
- 4 Kepler GPUs
- Now also AMG!



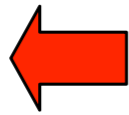
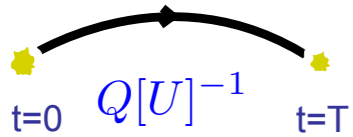
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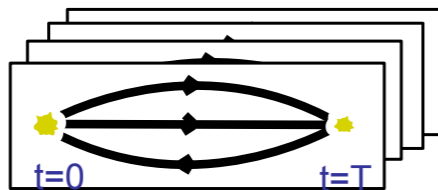
Contract

- 8 cores, CPUs



Correlators

100K – 1M copies



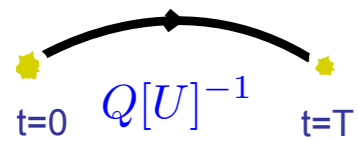
LQCD workflow

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Propagators



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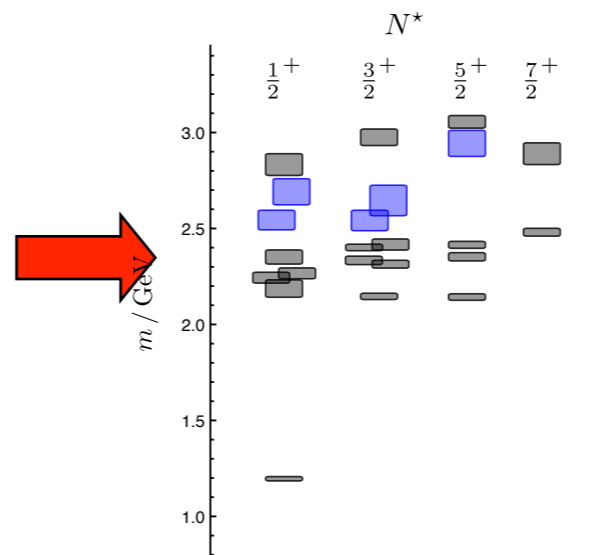
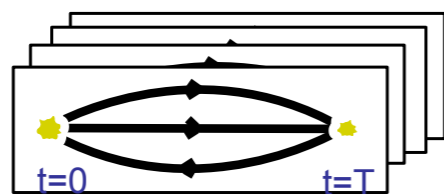
Contract

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Correlators

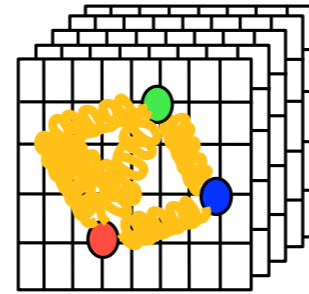
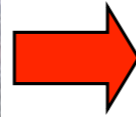
100K – 1M copies



LQCD workflow

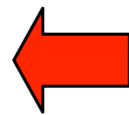
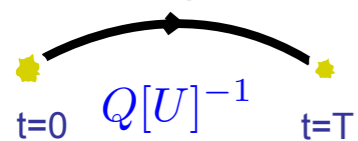
Generate the configurations

- Leadership level
- 60K cores, 10's TF-yr



Few big jobs
Few big files

Propagators



+



Analyze

100K copies
4 Kepler GPUs
Now also AMG!



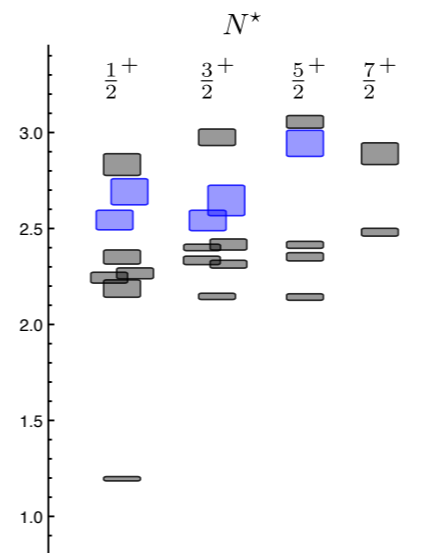
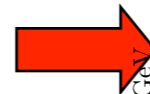
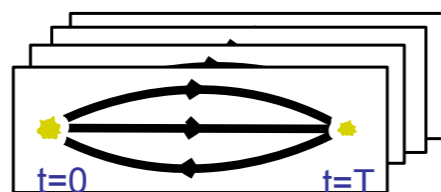
Contract

- 8 cores, CPUs



Correlators

100K – 1M copies



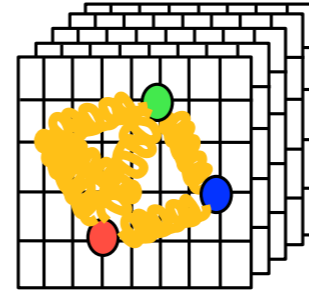
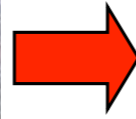
Many small jobs
Many big files

I/O movement

LQCD workflow

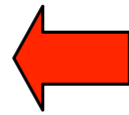
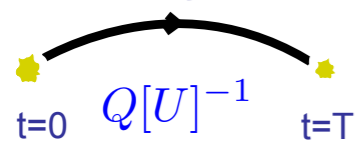
Generate the configurations

- Leadership level
- 60K cores, 10's TF-yr



~25%
Leadership level

Propagators



+



Analyze
100K copies
4 Kepler GPUs
Now also AMG!

~75%
Throughput mode

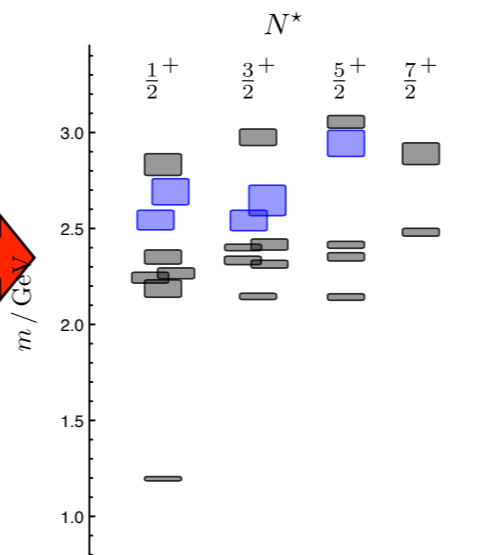
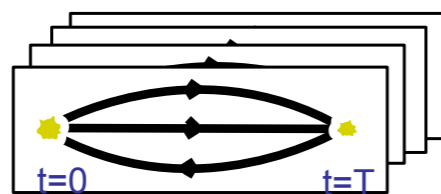
Contract

- 8 cores, CPUs



Correlators

100K – 1M copies



> 5%
New analysis cost

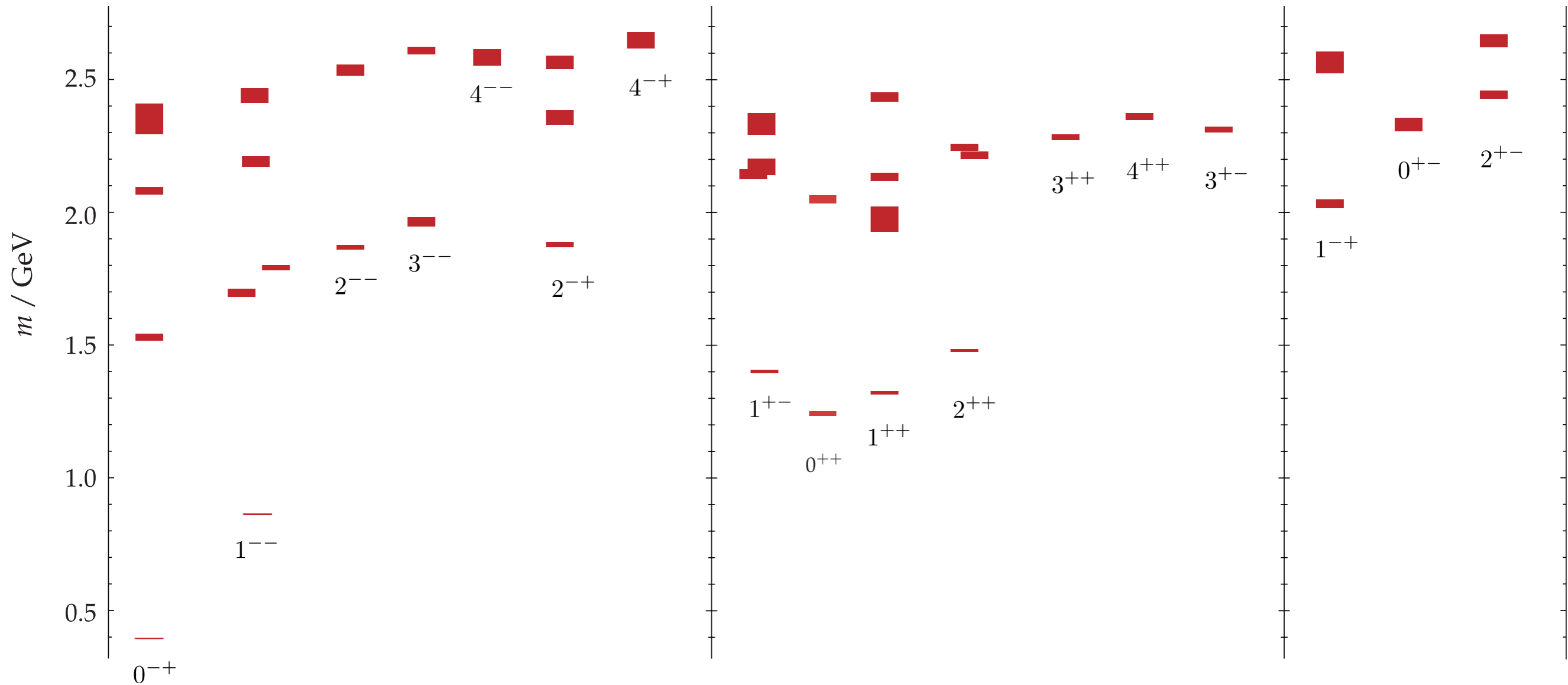
Leadership facilities & USQCD facilities

- Leadership resources - **capability**
 - Systems essential for USQCD gauge generation program
 - Networks + compute nodes designed to support large node count jobs
 - ➔ Titan: exchange rate is 20M core-hours for \$1M in integrated cost of project
 - DOE + NSF programs (INCITE, ALCC, Petascale) available for high profile critical applications
 - USQCD and associated projects quite successful
 - Highlight: JLab spectroscopy project: 250M core-hour project still largest award to date @ ORNL
- USQCD resources - **capacity**
 - Provide essential leverage of capability resources
 - Systems cost optimized for USQCD physics program
 - SciDAC essential to exploit new computing architectures
 - Virtuous circle - success at optimizing enables optimal use of future leadership systems
- JLab:
 - Improving energy efficiency of computing center - part of \$27M DOE project
 - Increasing power & cooling to support future growth in LQCD & 12GeV program
 - Developing resource sharing between Expt. Phys. & LQCD for increased utilization

Spectroscopy: isovector meson spectrum

- Appears to be some $q\bar{q}$ -like near-degeneracy patterns

$m_\pi \sim 391 \text{ MeV}$

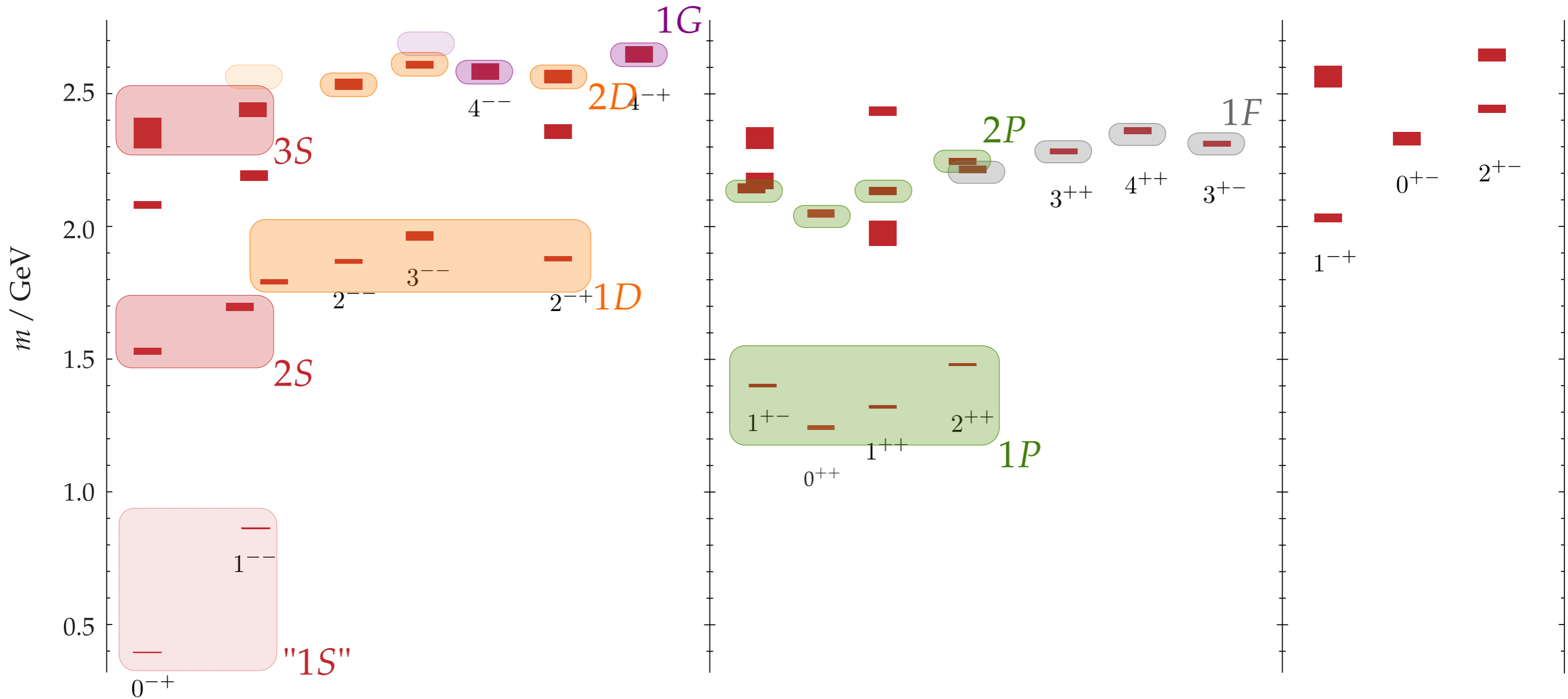


PRL 103; PRD 82, 88

Spectroscopy: isovector meson spectrum

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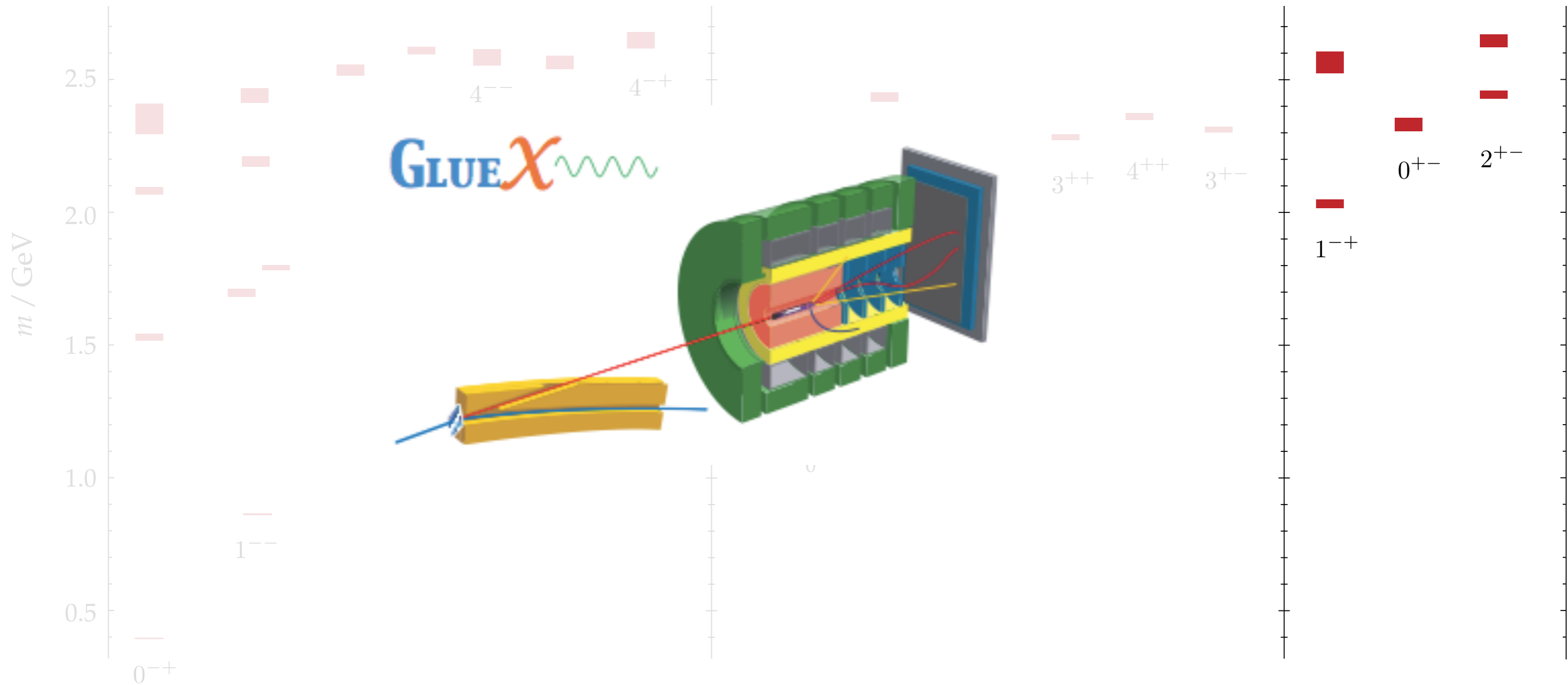


PRL 103; PRD 82, 88

Meson spectrum from lattice QCD

Multiple exotic mesons within range of GlueX

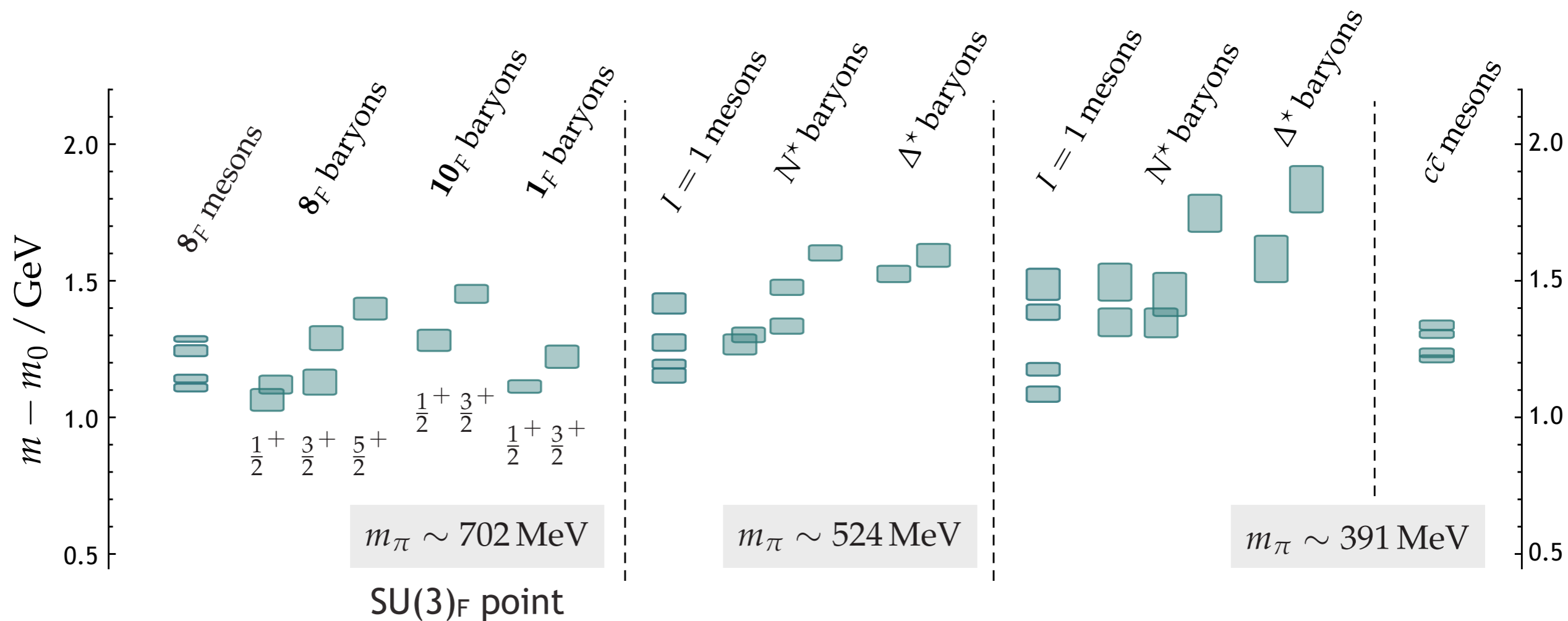
EXOTIC MESONS



PRL 103; PRD 82, 88

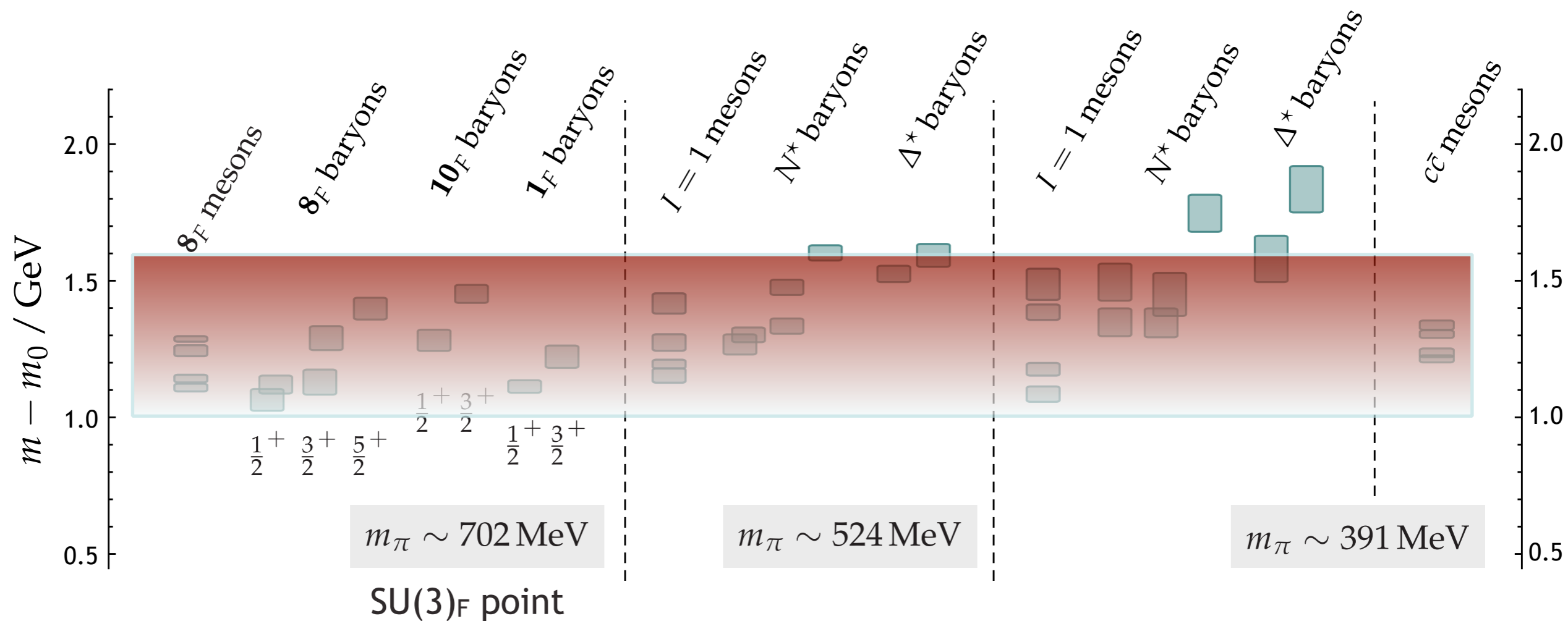
Chromo-magnetic excitation

- Subtract the 'quark mass' contribution



Chromo-magnetic excitation

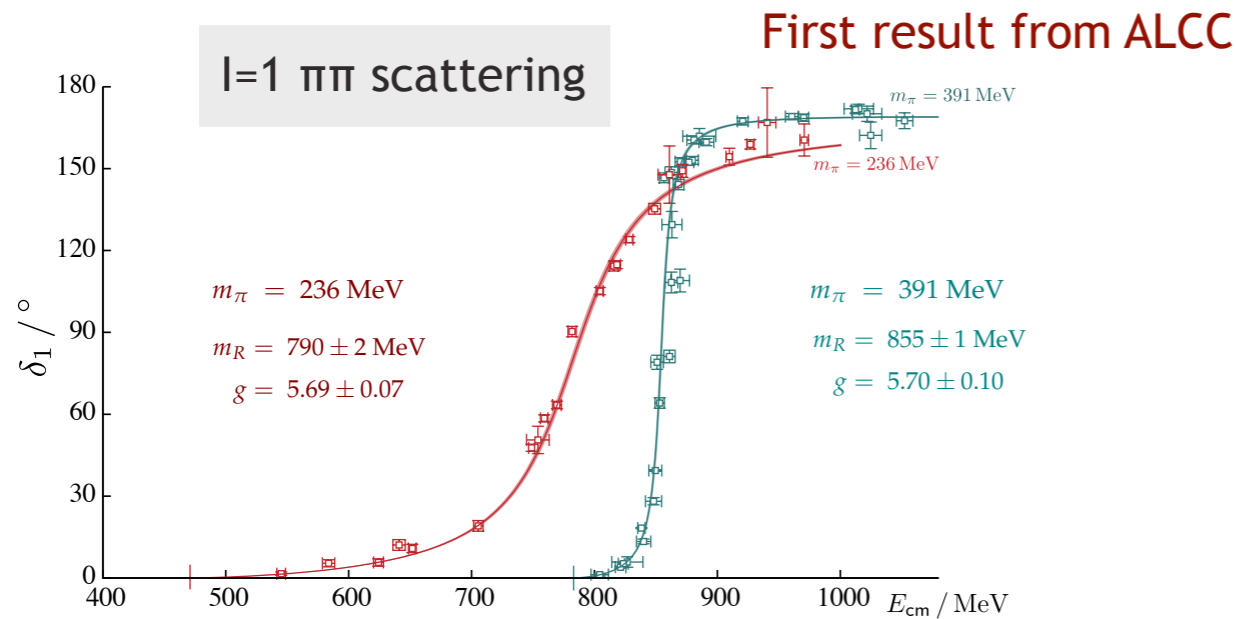
- Subtract the 'quark mass' contribution



– *Common energy scale of gluonic excitation* ~ 1.3 GeV

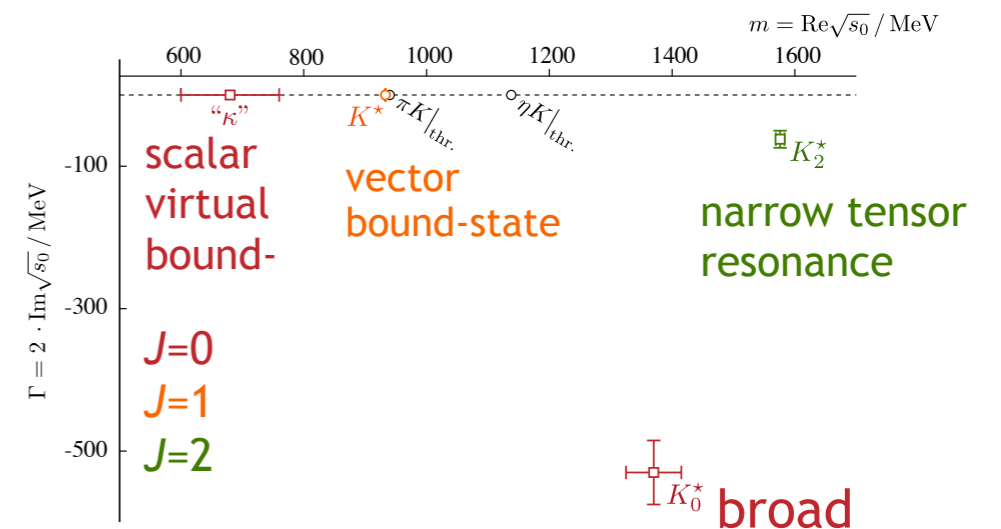
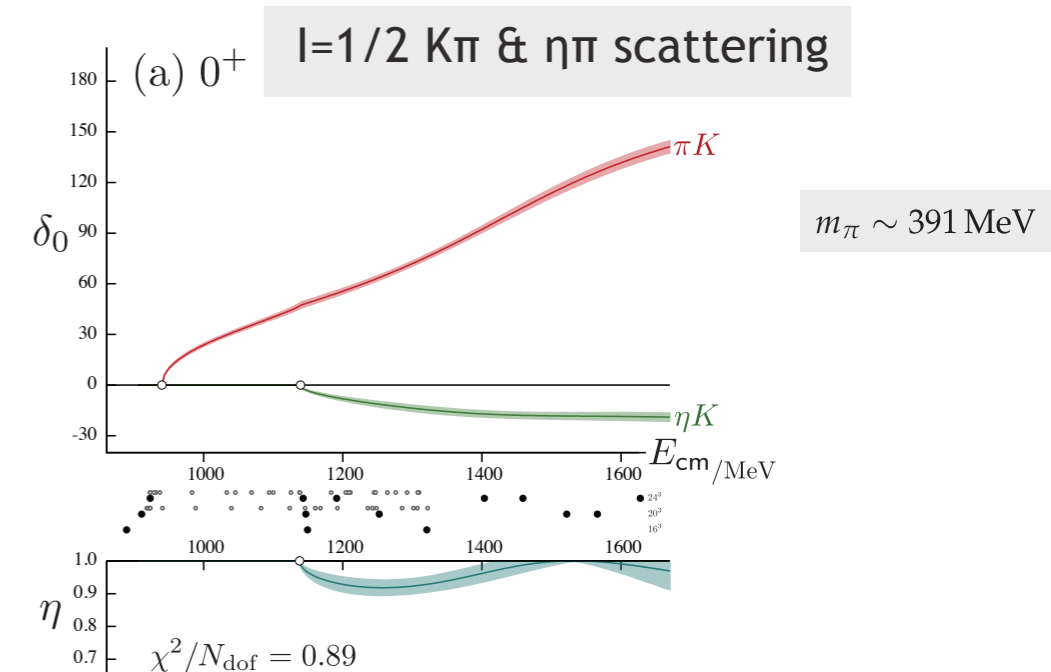
Spectroscopy

- First glimpse of spectrum of QCD light quark, strange quark, and charm quark mesons & baryons
- Results suggest rich pattern of states similar to non-rel. quark model + gluonic excitations
 - Possibly many states within energy range of GlueX
- Expt. verification requires measurement in many decay channels
 - Need partial wave couplings and resonance parameters



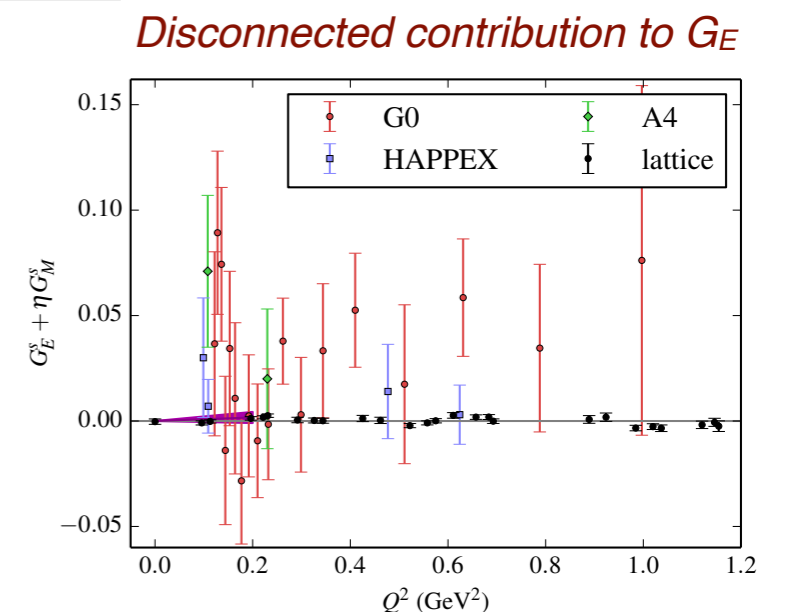
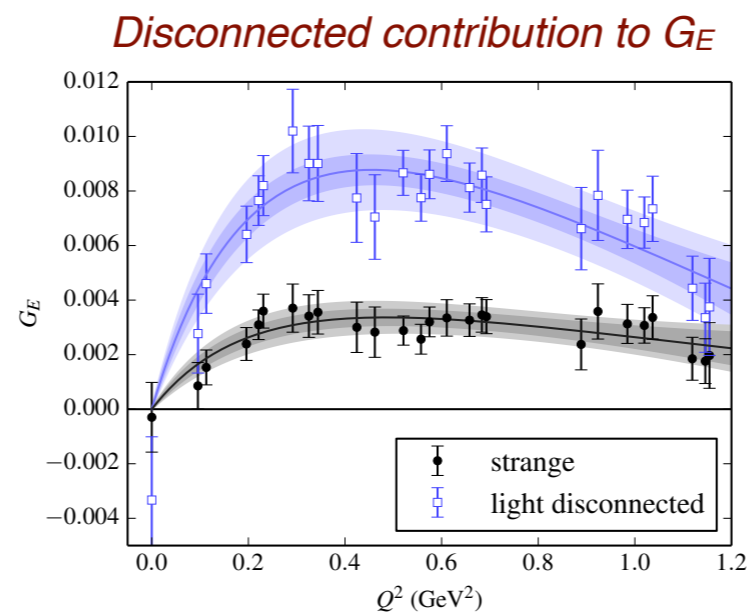
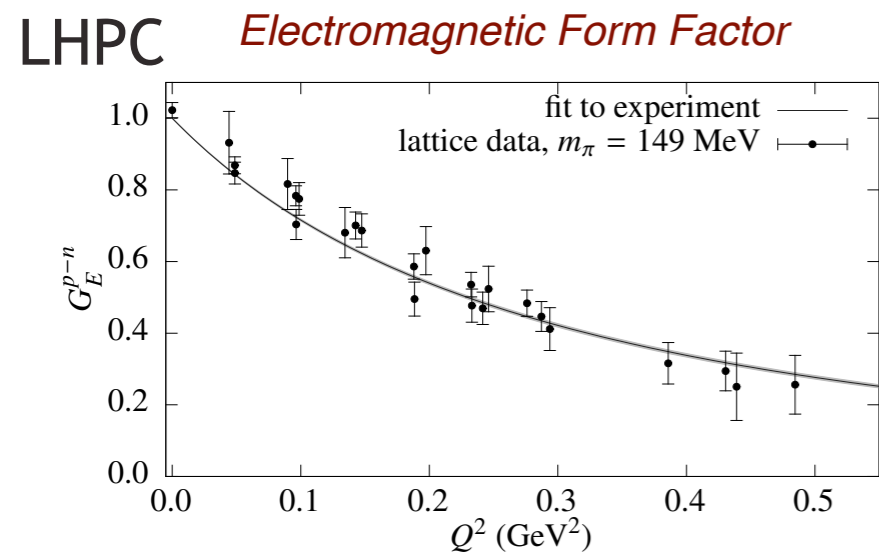
- First LQCD determination of coupled channel resonance
- Interesting observations about scalar sector
- Stepping stone to compute exotic meson parameters

PRL 113 182001
 PRD 91 054008
 1507.02599



Hadron Structure

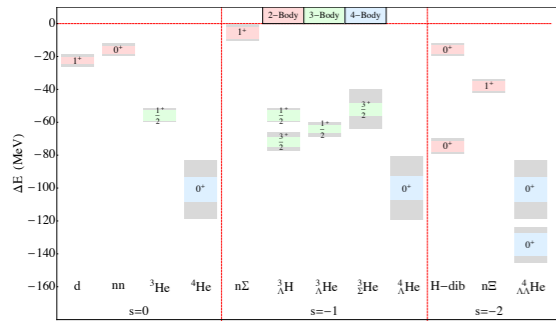
- LHPC: calc. @ $m_\pi=149$ MeV showing *isovector* $G_E(Q^2)$ and $G_M(Q^2)$ agree with expt. error band
 - Needed is the isoscalar contribution
- First calculation of disc. light quark contributions to EM form factors: $\sim 0.5\%$ of connected result
- Strange EM form factors consistent with expt. and much smaller uncertainty
 - *Hierarchical Probing* proved crucial to reduce noise by 10x and resolve the signal
- Challenge: to control systematic errors sufficiently to resolve proton radius puzzle



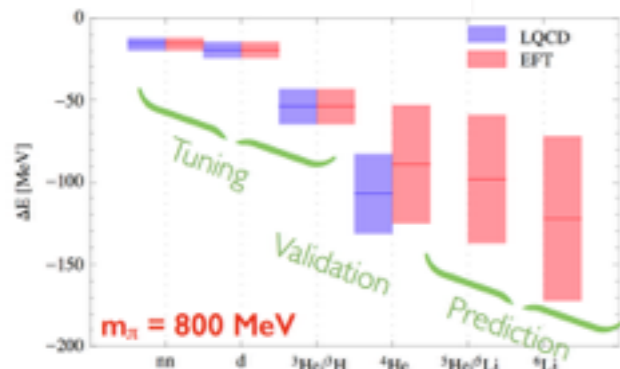
» S. Syritsyn will join JLab as a Nathan Isgur Fellow this fall

Orginos, Syritsyn + LHPC: 1404.4029, 1505.01803

Nuclear structure



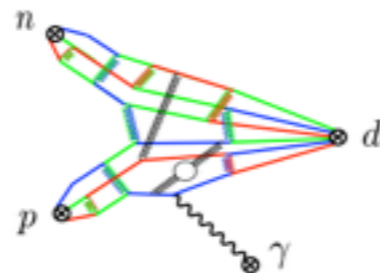
Nuclear Structure



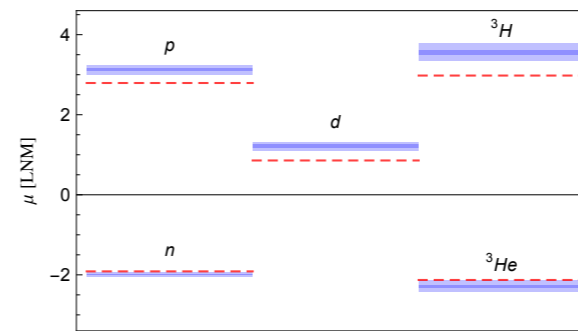
Refining Nuclear Forces

The binding of light nuclei and their properties

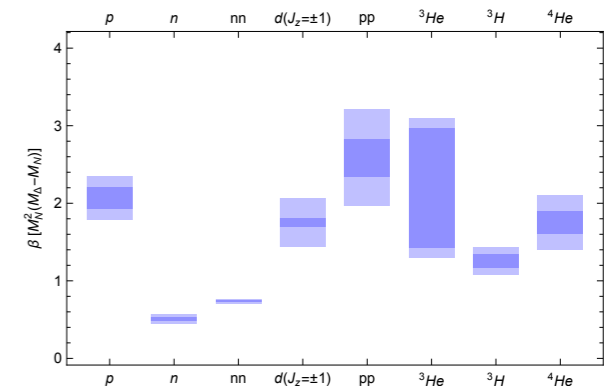
- Binding of light nuclei
 - Used to predict properties of larger nuclei through matching to Nuclear EFT
- First calculations of an inelastic nuclear reaction (neutron capture cross section)
- First calculations of the magnetic moments and polarizabilities of light nuclei
- ➔ Nuclear shell-model structure of light nuclei persists over range of quark masses
- ➔ Magnetic moments of nucleons are generically quark-model



Nuclear Reactions



Magnetic Moments



Nuclear Polarizabilities

Near Future Program:

- Properties of multi-neutron systems and the three-body forces
- Axial couplings for neutrino int. with nuclei
- Refinement of nuclear shell-model calculations of double beta-decay rates
- Nuclei and exotic nuclei at lighter pion masses

Orginos & NPLQCD: 1206.5219, 1301.5790, 1409.3356, 1505.02422, 1506.05518

Involvement with experimental program

Physics Opportunities with the 12 GeV Upgrade at Jefferson Lab

Jozef Dudek, Rolf Ent, Rouven Essig, Krishna Kumar, Curtis Meyer, Robert McKeown, Zein Eddine Meziani, Gerald A. Miller, Michael Pennington, David Richards, Larry Weinstein, Glenn Young

Second phase of GlueX program with BaBar DIRC-s (approved)

A study of decays to strange final states with GlueX in Hall D using components of the BaBar DIRC

(A proposal to the 42nd Jefferson Lab Program Advisory Committee)

M. Dugger,¹ B. Ritchie,¹ I. Senderovich,¹ E. Anassontzis,² P. Ioannou,² C. Kourkouveli,² G. Vasileiadis,² G. Voulgaris,² N. Jarvis,³ W. Levine,³ P. Mattione,³ W. McGinley,³ C. A. Meyer,³ R. Schumacher,³ M. Staib,³ F. Klein,⁴ D. Sober,⁴ N. Sparks,⁴ N. Walford,⁴ D. Doughty,⁵ A. Barnes,⁶ R. Jones,⁶ J. McIntyre,⁶ F. Mokaya,⁶ B. Pratt,⁶ W. Boeglin,⁷ L. Guo,⁷ E. Pooser,⁷ J. Reinhold,⁷ H. Al Ghoul,⁸ V. Crede,⁸ P. Eugenio,⁸ A. Ostrovidov,⁸ A. Tsaris,⁸ D. Ireland,⁹ K. Livingston,⁹ D. Bennett,¹⁰ J. Bennett,¹⁰ J. Frye,¹⁰ M. Lara,¹⁰ J. Leckey,¹⁰ R. Mitchell,¹⁰ K. Moriya,¹⁰ M. R. Shepherd,¹⁰ O. Chernyshov,¹¹ A. Dolgolenko,¹¹ A. Gerasimov,¹¹ V. Goryachev,¹¹ I. Ladin,¹¹ V. Matveev,¹¹ V. Tarasov,¹¹ F. Barbosa,¹² E. Chudakov,¹² M. Dalton,¹² A. Deur,¹² J. Dudek,¹² H. Egiyan,¹² S. Furletov,¹² M. Ito,¹² D. Mack,¹² D. Lawrence,¹² M. McCaughan,¹² M. Pennington,¹² L. Pentchev,¹² Y. Qiang,¹² E. Smith,¹² A. Somov,¹² S. Taylor,¹² T. Whitlatch,¹² B. Zihlmann,¹²

Science case for JLab CLAS12 expt (approved)

Studies of Nucleon Resonance Structure in Exclusive Meson Electroproduction

I. G. Aznauryan,^{1,2} A. Bashir,³ V. M. Braun,⁴ S. J. Brodsky,^{5,6} V. D. Burkert,² L. Chang,^{7,8} Ch. Chen,^{7,9,10} B. El-Bennich,^{11,12} I. C. Cloët,^{7,13} P. L. Cole,¹⁴ R. G. Edwards,² G. V. Fedotov,^{15,16} M. M. Giannini,^{17,18} R. W. Gothe,¹⁵ F. Gross,^{2,19} Huey-Wen Lin,²⁰ P. Kroll,^{21,4} T.-S. H. Lee,⁷ W. Melnitchouk,² V. I. Mokeev,^{2,16} M. T. Peña,^{22,23} G. Ramalho,²² C. D. Roberts,^{7,10} E. Santopinto,¹⁸ G. F. de Teramond,²⁴ K. Tsushima,^{13,25} and D. J. Wilson^{7,26}

Involvement with experimental program

NSAC report prominently features spectroscopy, hadron and nuclear structure projects

Report to the
Nuclear Science Advisory Committee
Implementing the 2007 Long Range Plan
January 31, 2013

Looking towards the future - community

Town Hall report providing input to next NSAC Long Range Plan

Computational Nuclear Physics Meeting SURA Headquarters, Washington DC, July 14-15, 2014

REPORT

Prepared by the Computational Nuclear Physics Meeting Writing Committee
**A. Burrows, J. Carlson, W. Detmold, R. Edwards, R. Furnstahl, F. Karsch,
W. Nazarewicz, P. Petreczky, D. Richards, W. Hicks, M.J. Savage.**

Recommendations endorsed at Joint Town Meeting on QCD in 2014

» New NSAC report in preparation now...

Looking towards the future - software

Proposals for coordinated software development for next generation Leadership Computing Facilities

NERSC: Chroma Lattice QCD Code Suite, Balint Joo (Jefferson National Accelerator Facility)

Center for Accelerated Application Readiness: Preparing USQCD Lattice Gauge Theory Codes for Readiness on Summit

Primary PI: Robert G. Edwards
Senior Staff Scientist
Thomas Jefferson National Accelerator Facility (Jefferson Lab)
Email: edwards@jlab.org, *Phone:* (757) 269-7737

Oak Ridge:

Co-PIs:

Bálint Joó
Staff Scientist
Jefferson Lab
Email: bjoo@jlab.org
Phone: (757) 269-5339

Richard C. Brower
Physics Department
Boston University
Email: brower@bu.edu
Phone: (617) 353-6052

Steven A. Gottlieb
Department of Physics
Indiana University
Email: sg@indiana.edu
Phone: (812) 855-0243

Chulwoo Jung
Department of Physics
Brookhaven National Laboratory
Email: chulwoo@bnl.gov
Phone: (631) 344-5254

Michael A. Clark
NVIDIA Corporation
Email: mclark@nvidia.com
Phone: (617) 820-4824

Argonne: The Hadronic Contribution to the Anomalous Magnetic Moment of the Muon
Co-PI: Balint Joo (porting Chroma to “Theta” at ANL)

Looking towards the future - science program

- Spectroscopy
 - Suggests rich spectrum of mesons & baryons - exotic & non-exotic hybrids
 - Next phase:
 - multi-meson (3 or more) scattering
 - tackle two-quark exotics & scalar sector
 - tetra-quarks - charm, strange, then light
 - N^* and strange-baryon spectrum and decays
- Hadron structure
 - First calculations at phys. pion mass of isovector quantities - charge radius, moments...
 - Next phase:
 - direct calculation of isoscalar quantities - resolve proton charge radius “puzzle”
 - full decomposition of spin from quarks and glue - relevant for 12GeV
 - direct determination of quark distributions from pseudo-distributions (Ji’s method)
 - structure of excited states gives insight into glue distribution - relevant to EIC
- Nuclear structure
 - First predictions for larger nuclei through matching to nuclear EFT
 - Next phase:
 - multi-neutron systems and three-body forces
 - axial couplings for neutrino interactions & refinement of double beta-decay rates

Looking towards the future - resources

- Ambitious program - however, constrained by available computational and manpower resources
- Increase in computing resources:
 - Coordination via NSAC process
 - Regain lost share in USQCD facilities funding
 - NSF
- Increase in manpower resources
 - SciDAC - computational expertise
 - Recognize that S-matrix formalism & phenomenology increasingly important
 - DOE Topical collaborations
 - More collaborations in phenomenology
 - NSF

Backup slides

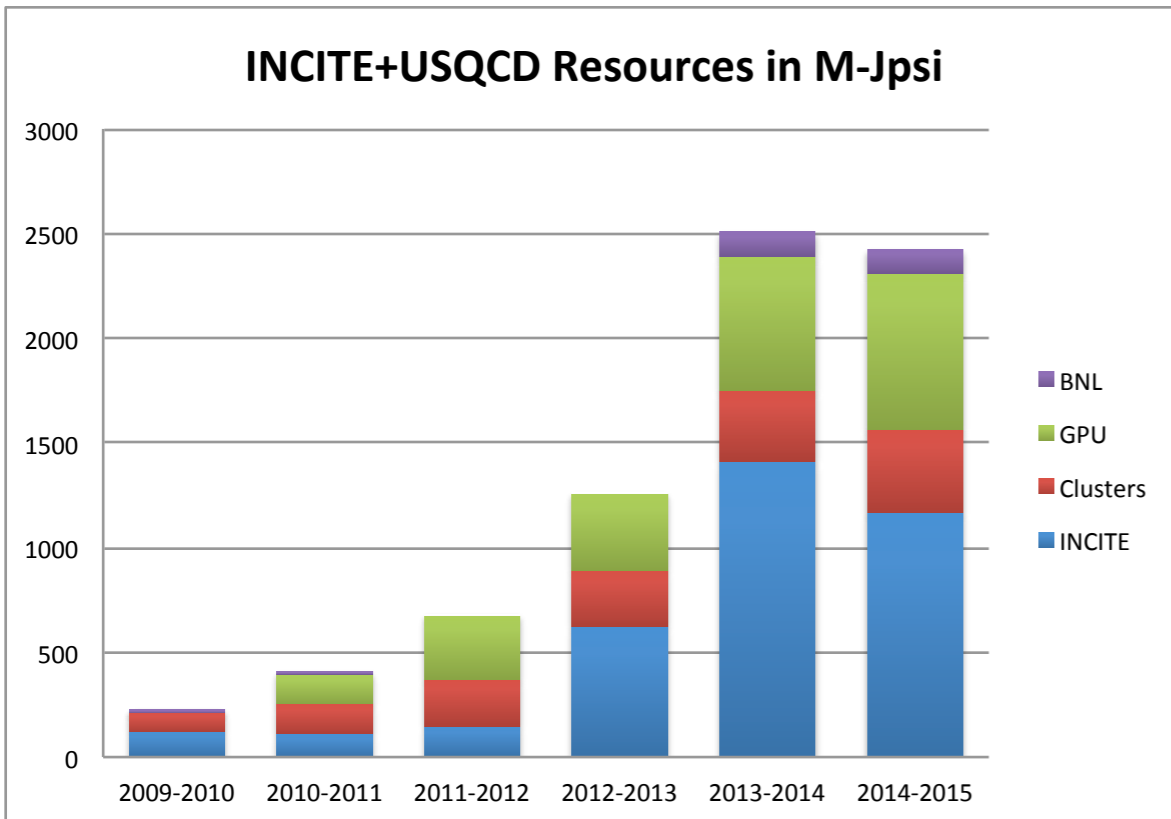
USQCD + INCITE computing resources

Comparison of computing resources available to USQCD (in Million core-hours)

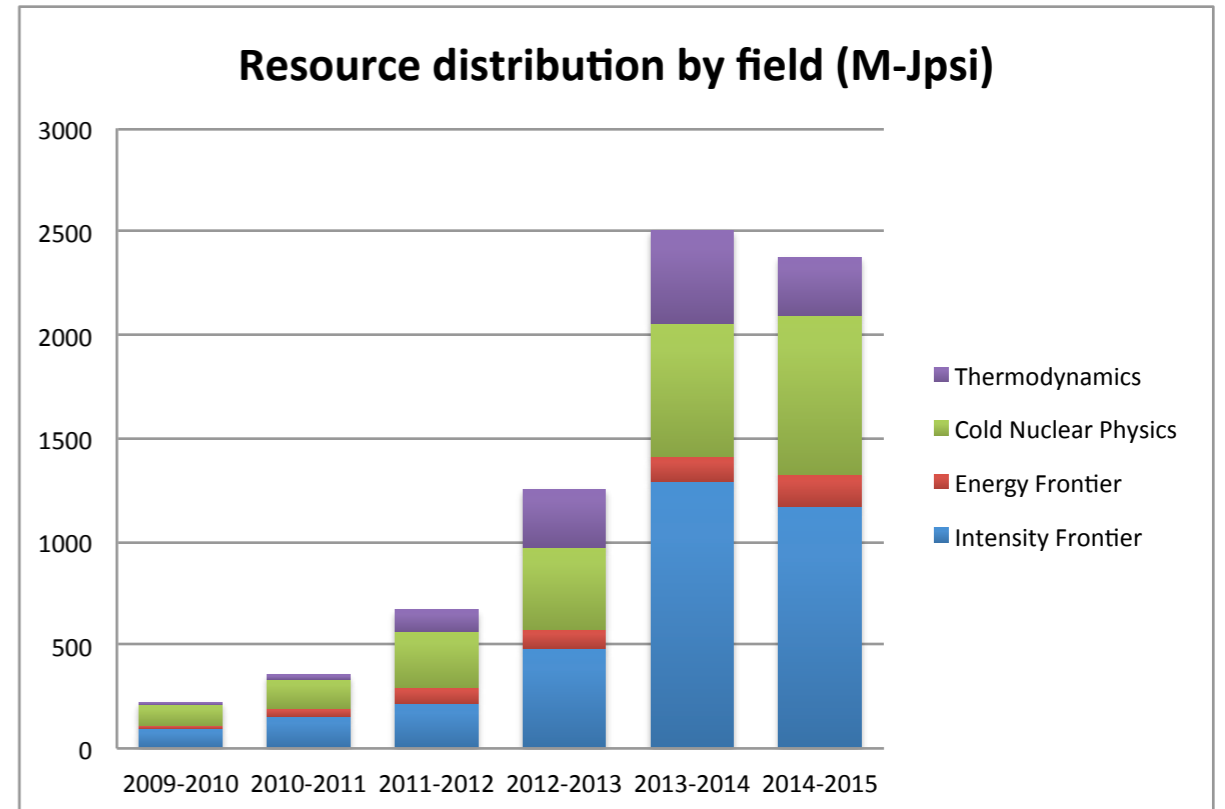
Normalize by LQCD performance over different machines/performances

A “Jpsi” is a unit based on a ~2010 CPU architecture with 100M Jpsi core-hours = 14 TF-yr

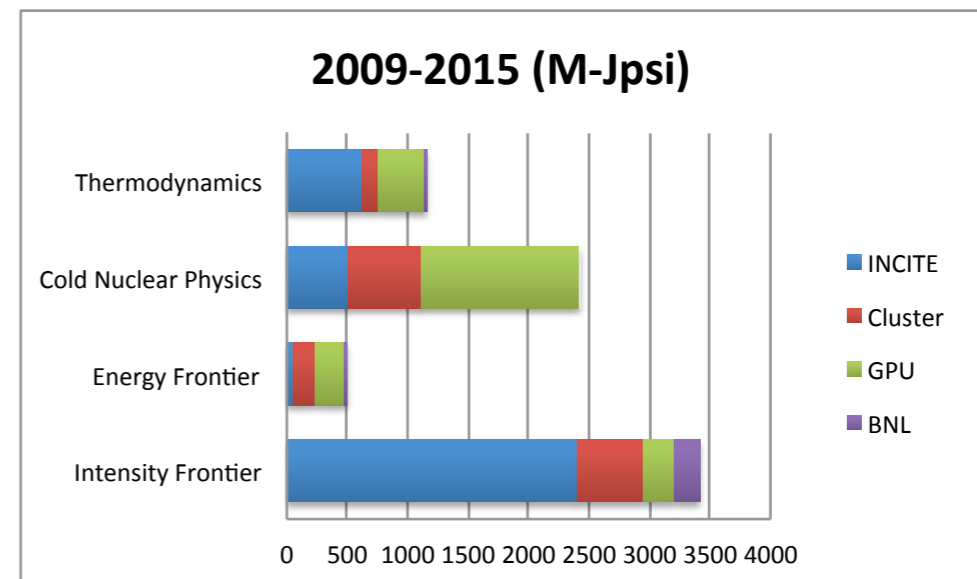
INCITE+USQCD Resources in M-Jpsi



Resource distribution by field (M-Jpsi)



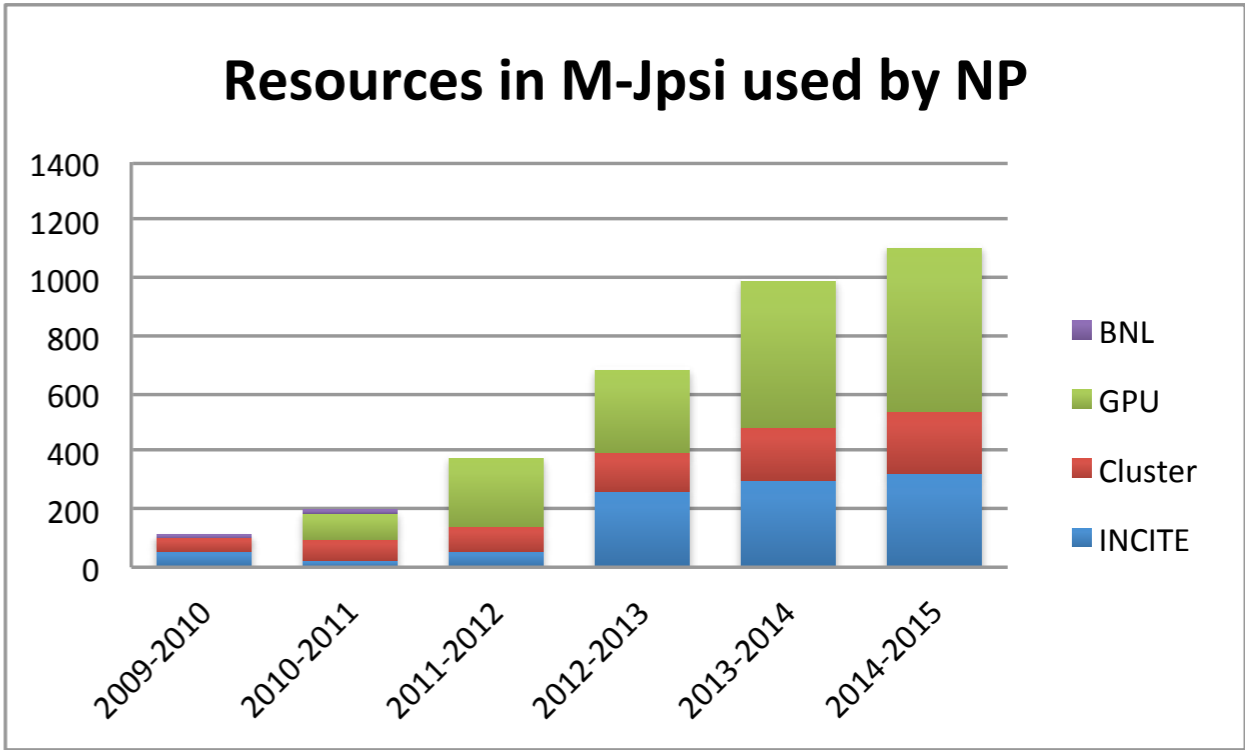
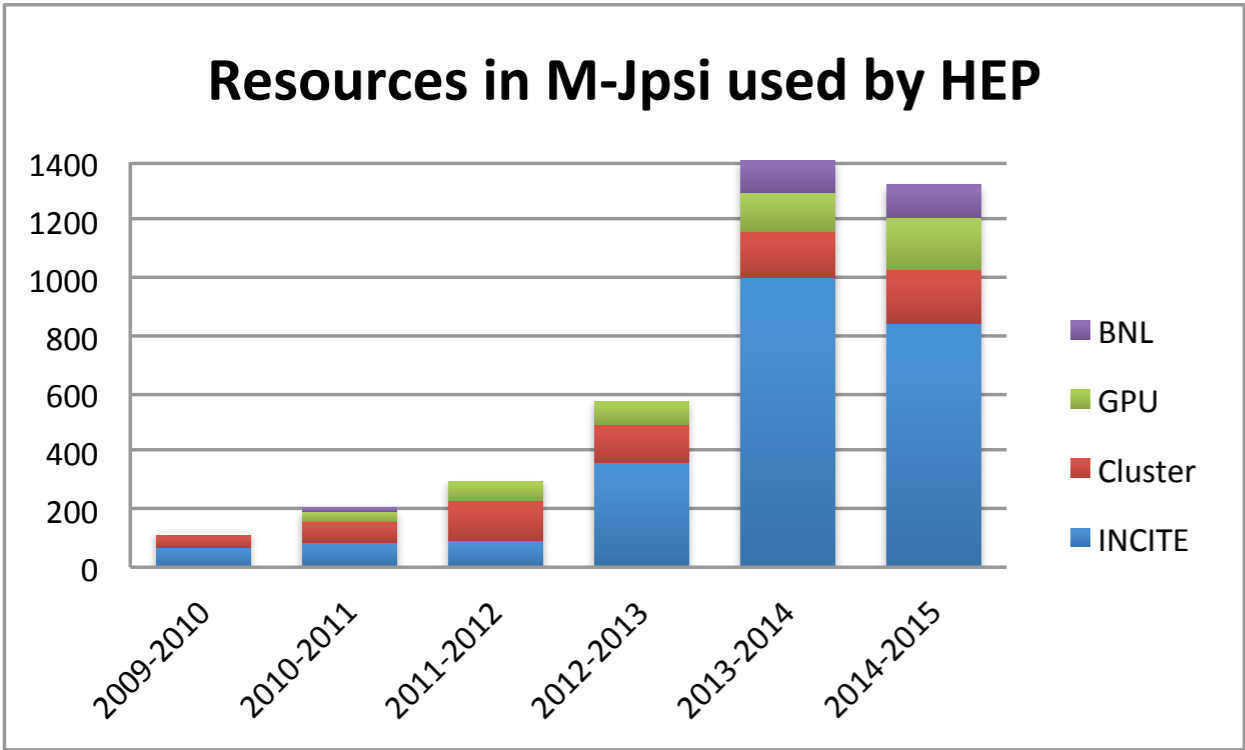
2009-2015 (M-Jpsi)



USQCD + INCITE computing resources

Comparison of computing resources available to USQCD (in Million core-hours)

NP receives the majority of its flops from USQCD resources



Excited states from correlators

- How to get at excited QCD eigenstates ?

- optimal operator for state $|\mathbf{n}\rangle$ $\Omega_{\mathbf{n}}^{\dagger} \sim \sum_i v_i^{(\mathbf{n})} \mathcal{O}_i^{\dagger}$

for a basis of meson operators $\{\mathcal{O}_i\}$

- can be obtained (in a variational sense) from the matrix of correlators

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t) \mathcal{O}_j^{\dagger}(0) | 0 \rangle$$

- by solving a generalized eigenvalue problem

$$C(t)v^{(\mathbf{n})} = C(t_0)v^{(\mathbf{n})} \lambda_{\mathbf{n}}(t)$$

eigenvalues

$$\lambda_{\mathbf{n}}(t) \sim e^{-E_{\mathbf{n}}(t-t_0)}$$

‘diagonalize the correlation matrix’

- a large basis can be constructed using covariant derivatives :

$$\mathcal{O} \sim \bar{\psi} \Gamma \overleftrightarrow{D} \dots \overleftrightarrow{D} \psi$$

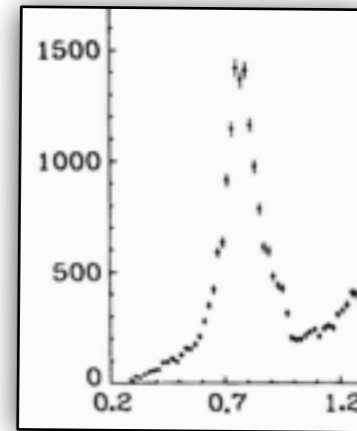
Contraction costs - 2015

	T	$t = 0$		Cost: $N \propto$ Volume	Assuming dense tensors
Meson spectroscopy meson			$\text{tr}(MPMP)$	$\sim N^3$	easy
meson-meson				orientations $\sim 100 \times N^3$	affordable
tetraquark				$\sim N^5$	sparse in spin, but not really affordable
Hadron structure baryon				$\sim N^4$	affordable
Baryon spectroscopy baryon-meson				$\sim 100 \times N^4$	to do a decent job, not affordable
pentaquark				$\sim N^6$	prohibitive

ρ resonance - a comparison of techniques

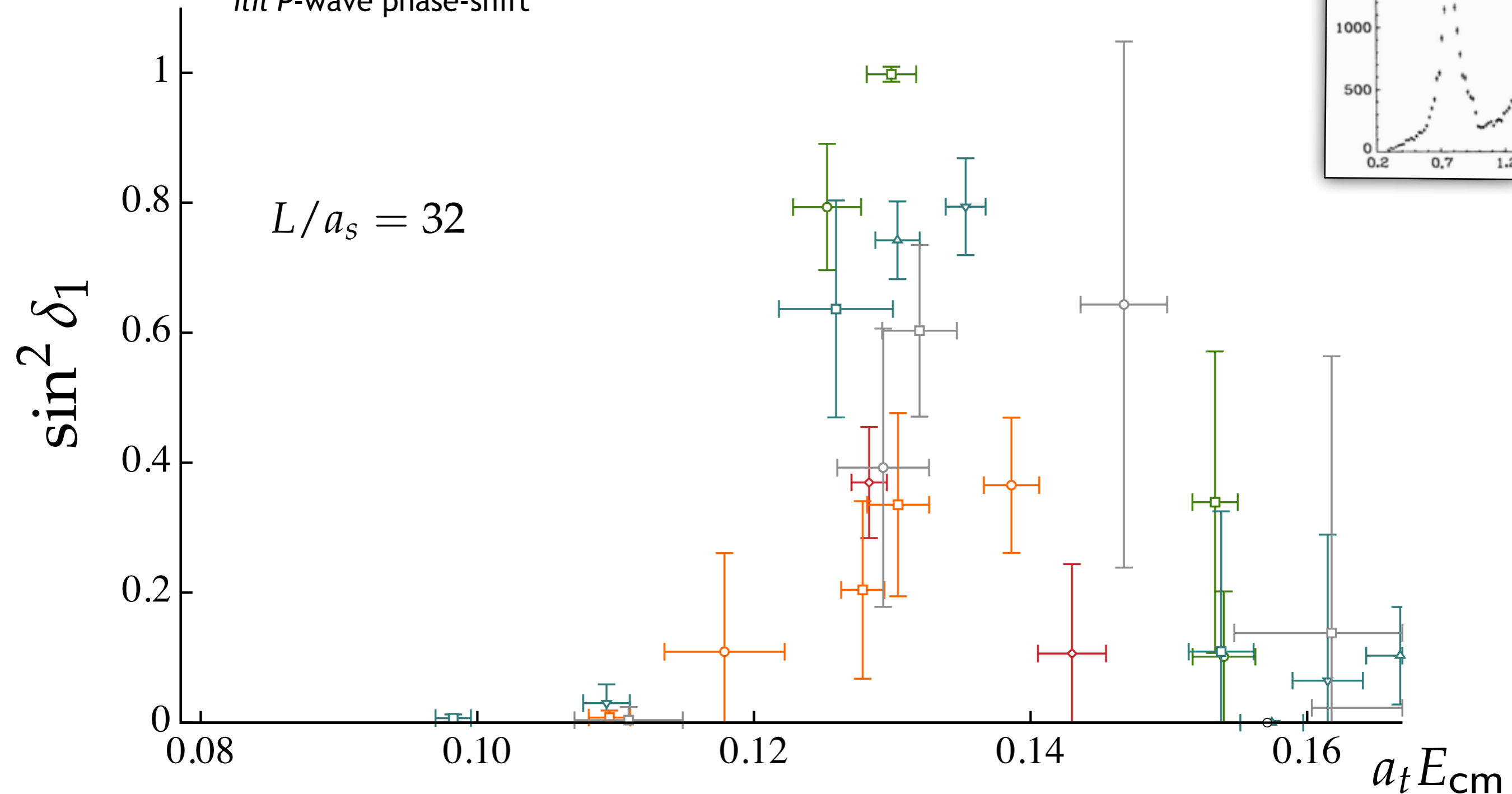
$m_\pi \sim 230 \text{ MeV}$

(Cheaper) Stochastic method



$\pi\pi$ P-wave phase-shift

$L/a_s = 32$

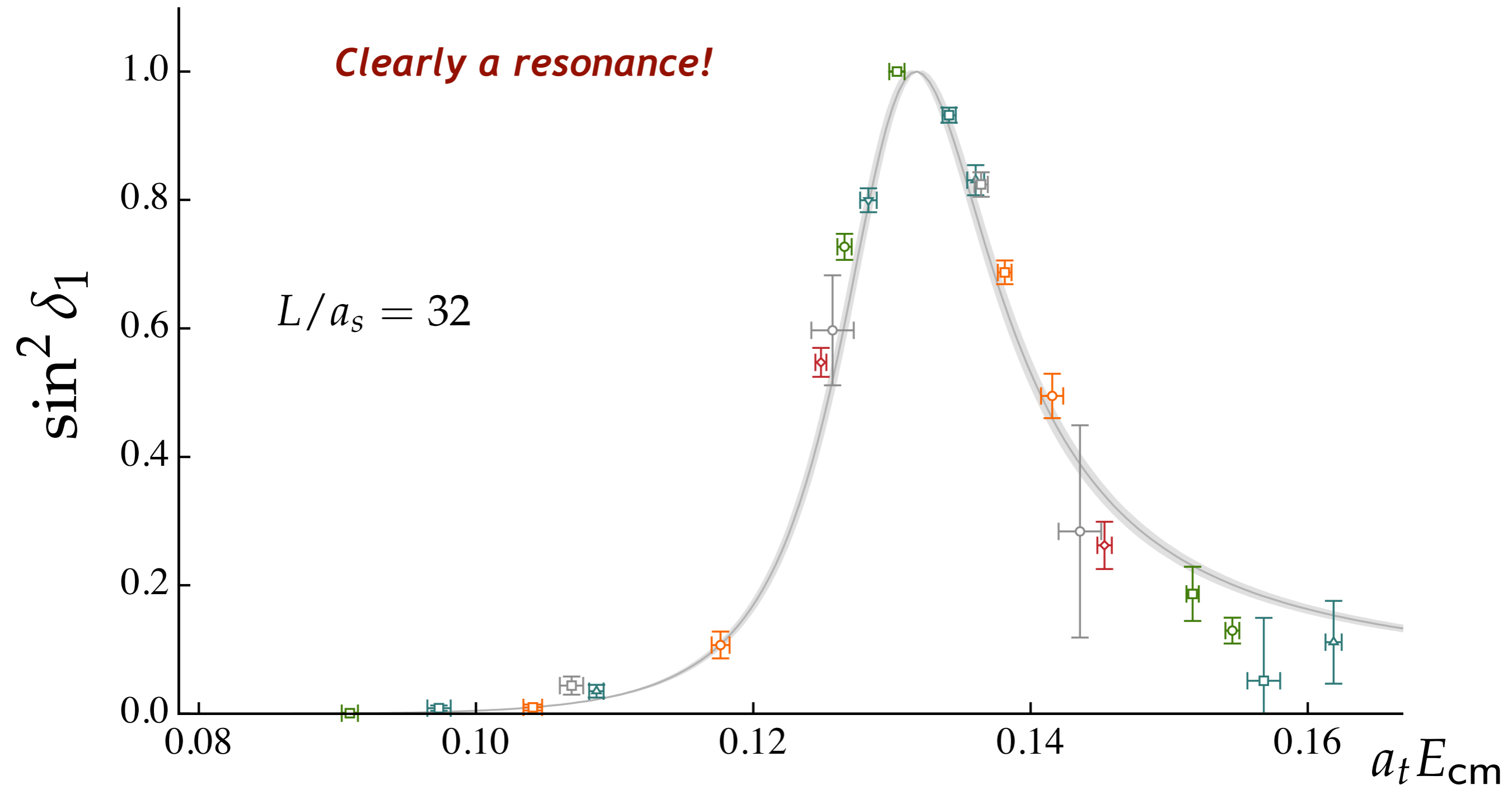


Fahy, et.al. arXiv:1410.8843

Result of ALCC

$m_\pi \sim 230 \text{ MeV}$

Full distillation method

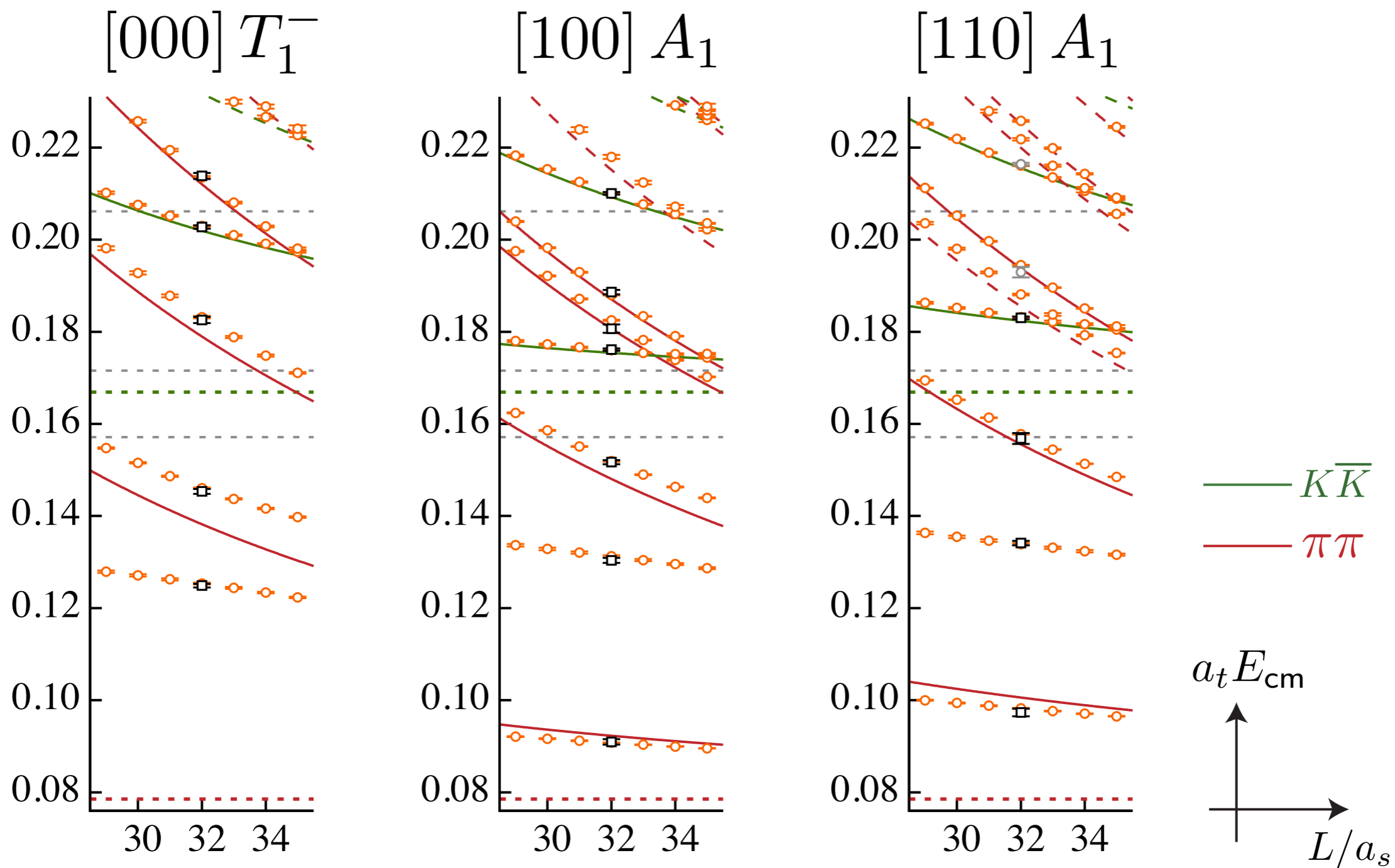


HadSpec: 1507.02599

$\pi\pi/K\bar{K}$ scattering - “ ρ ”

$m_\pi \sim 236$ MeV

- Data points (black) compared to parameterization (gold)



HadSpec: 1507.02599

$\eta\pi/KK$ scattering - “a0”

$m_\pi \sim 391$ MeV

- Precision (< 1%) essential in constraining scattering levels

